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Wed. 02. 09., 10⁴⁰-11⁰⁰

SAXS studies of selected flexible proteins or proteins of modular structure

Wed. 02. 09., 11⁴⁰-12²⁰

High-brilliance X-ray sources: a bright future for life science studies

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Keywords: synchrotron radiation, free electron laser, life sciences

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More than twenty years ago, a wide access to 3rd generation synchrotron radiation (SR) sources has brought an accelerated growth in studies of a condensed matter. Unique properties of SR together with countless improvements both in the experimental and computational techniques have also opened up new exciting era, especially in research of the biological structures and processes. A variety of methods employed to study biological matter on the levels from molecules through cells and tissues up to whole organisms, like X-ray crystallography, spectroscopies in a broad range of wavelengths from IR up to hard X-rays, a number of imaging techniques, and many other, have led to a substantial progress in the life science and related fields.

The history repeats over the last decade, due to a rapid development of the short-wavelength Free Electron Lasers (FELs), new 4th generation SR sources. They can produce a fully tunable monochromatic radiation, including hard X-rays, in ultrafast femtosecond pulses with a peak power up to several GW. FELs break fundamental barriers that limit all other known X-ray sources. This means new marvelous qualities in probing the secrets of life with unprecedented femtosecond temporal and atomic spatial resolution. With FELs, it is possible to study even single macromolecules using enormously large, damaging irradiation doses and acquire structural information before the object is damaged. In this way one can explore both crystals and small nanocrystals and noncrystalline materials.

This talk is aimed at showing, in a short trip across fascinating areas of high-brilliance X-ray sources, how plainly is emerging the brightest ever future for experimental methods. The perspectives emerging from having to be opened soon the first Polish synchrotron, SOLARIS, as well as the access to the EU-XFEL facility in Hamburg, the project developed with participation of Poland will be also mentioned.

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Keywords: synchrotron radiation, small angle X-ray scattering, disordered proteins, modular structure

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Small angle scattering of synchrotron radiation (SR-SAXS) is a technique, which is suitable to the study of difficult biomacromolecules, and especially the low resolution structure in solution of the proteins possessing the flexible or modular structure. Due to the flexibility of the conformation of these macromolecules, is very difficult (or nearly impossible) to obtain their atomic structures based on the classic methods of protein crystallography. On the other hand, these proteins often play important physiological functions in which a flexible conformation of the protein molecule is crucial for the its function (in regulation, signaling and control pathways) [1]. The physiological function of flexible proteins often is complementary to function played by other ordered protein molecules or protein domains [2,3]. Therefore is very important to have in our disposal a routine method dedicated to the determination of flexible structures in solution.

SAXS technique also offers also a substantial support in the prediction and modelling of protein structure by the use of bioinformatics. Low resolution structural protein models in solution, obtained by SAXS, can be used as templates (molecular envelopes) for docking of bioinformatics models [4]. As a result, the full molecular structures, even large proteins or protein complexes, can be determined [5].

In recent years, SAXS is also used in other applications, including also the use of low resolution models to verify NMR structures, or even in supplementation the NMR data [6].

During the lecture will be presented the applications of SR-SAXS technique in the study of selected disordered protein systems, modular proteins, protein complexes, denaturation processes as well as the conformational dynamics of macromolecules in solution. Special attention will be paid on proteins from plant innate defence systems [7], regulatory proteins and on the conformational dynamics of proteins involved in neurodegenerative diseases [8].

Acknowledgments: This research project has been financed by the funds from the National Science Centre (Poland) granted on the basis of decision no. DEC-2012/06/M/ST4/00036.

^[1] V. N. Uversky, *Biochimica et Biophysica Acta* **1834** (2013) 932.